

# 2-Butenedioic acid (e), dioctyl ester

<b>Inchi:</b>	InChI=1S/C20H36O4/c1-3-5-7-9-11-13-17-23-19(21)15-16-20(22)24-18-14-12-10-8-6-4-2
<b>InchiKey:</b>	TVWTZAGVNBXPXHU-FOCLMDBBSA-N
<b>Formula:</b>	C20H36O4
<b>SMILES:</b>	CCCCCCCCOC(=O)C=CC(=O)OCCCCCCCC
<b>Mol. weight [g/mol]:</b>	340.50
<b>CAS:</b>	2997-85-5

## Physical Properties

Property code	Value	Unit	Source
gf	-270.10	kJ/mol	Joback Method
hf	-828.51	kJ/mol	Joback Method
hfus	53.33	kJ/mol	Joback Method
hvap	78.38	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.350		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1115.57	kPa	Joback Method
tb	813.74	K	Joback Method
tc	999.86	K	Joback Method
tf	454.40	K	Joback Method
vc	1.183	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.87	J/molxK	813.74	Joback Method
cpg	1022.58	J/molxK	968.84	Joback Method
cpg	1008.72	J/molxK	937.82	Joback Method
cpg	993.95	J/molxK	906.80	Joback Method
cpg	978.23	J/molxK	875.78	Joback Method
cpg	961.55	J/molxK	844.76	Joback Method
cpg	1035.55	J/molxK	999.86	Joback Method
dvisc	0.0000463	Paxs	813.74	Joback Method
dvisc	0.0000615	Paxs	753.85	Joback Method

dvisc	0.0000858	Paxs	693.96	Joback Method
dvisc	0.0001274	Paxs	634.07	Joback Method
dvisc	0.0002056	Paxs	574.18	Joback Method
dvisc	0.0003707	Paxs	514.29	Joback Method
dvisc	0.0007807	Paxs	454.40	Joback Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2997855&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2997855&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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